arXiv:cond-mat/9804314v1 [cond-mat.supr-con] 29 Apr 1998

The Low-Field Critical End Point of the First Order Transition Line in $YBa_2Cu_3O_{7-\delta}$

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(February 1, 2008)

We report on simulations of the first order phase transition in $YBa_2Cu_3O_{7-\delta}$ using the Lawrence-Doniach model. We find that the magnetization discontinuity vanishes and the first order transition line ends at a critical end point for low magnetic fields in agreement with experiment. The transition is not associated with vortex lattice melting, but separates two vortex liquid states characterized by different degrees of short-range crystalline order and different length scales of correlations between vortices in different layers.

PACS numbers: 74.20.De, 74.25.Dw, 74.25.Ha

Some features of the $B-T$ phase diagram of clean untwinned crystals of the high temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) are widely agreed upon. As the temperature is reduced the vortex liquid undergoes a first order phase transition to what is commonly assumed to be the Abrikosov vortex lattice state. There is striking experimental evidence for this first order transition. Sharp drops in resistivity [1,2] as well as discontinuities in magnetization and entropy [3,4] occur simultaneously and mark the transition line. A neglected feature of the experimental first order transition line in YBCO is its termination at low ($\approx 0.5T$) magnetic fields. This has been consistently observed in all relevant experiments (i.e. the latent heat, magnetization jump and sharp resistance drop all disappear for fields smaller than some lower critical field) [1–4]. Nevertheless the transition line is often shown extrapolated to T_c, because a transition which separates phases of different symmetries, like a vortex lattice and a vortex liquid, cannot simply disappear.

We report in this paper numerical results obtained for the Lawrence-Doniach (LD) [5] model for a clean superconductor which show that the low field end point of the transition is not an artifact due to disorder (as commonly thought) and that the interpretation of the first order transition as due to flux lattice melting must be incorrect. We see a first order liquid-liquid line with a critical end point at low fields, which in the $B-T$ phase diagram shown in Fig.1(a) agrees very well with the experimental YBCO "melting" line. On crossing the transition line, length and time scales increase discontinuously, but remain finite even in the low-temperature phase. The magnetization jumps we observe are shown in Fig.1(b) and are also in very good agreement with measurements in YBCO. Figure 1 is obtained using standard YBCO values for the fitting parameters; viz for the Landau-Ginzburg parameter κ=60, the mass anisotropy $\gamma=\sqrt{m_c/m_{ab}}$=7.5, the slope of the mean field transition line $\partial B_{c2}/\partial T|_{T=T_c} = -2$T/K, the mean field T_c=92.5K and the layer separation d=11.4Å. It is perhaps noteworthy that one of us has frequently expressed doubts regarding the vortex-lattice melting scenario [6,7] on the grounds that a finite temperature freezing to a flux lattice state is difficult to reconcile with the analytical result that off-diagonal long range order – a central feature of superconductivity – cannot coexist with a flux lattice at non-zero temperatures in three dimensions [7].

The LD model for a layered superconductor consists of a stack of planes with Josephson coupling between neighboring layers. With the superconducting order parameter in the n^{th} layer denoted as ψ_n, the Hamiltonian for the layered system with a magnetic field perpendicular to the layers is

$$\mathcal{H}= \sum_{n} d_0 \int d^2r \left(\alpha|\psi_n|^2 + \frac{\beta_{2D}}{2}|\psi_n|^4 + \frac{1}{2m_{ab}}|(-i\hbar\nabla - 2e\mathbf{A})\psi_n|^2 + J|\psi_{n+1}-\psi_n|^2 \right),$$

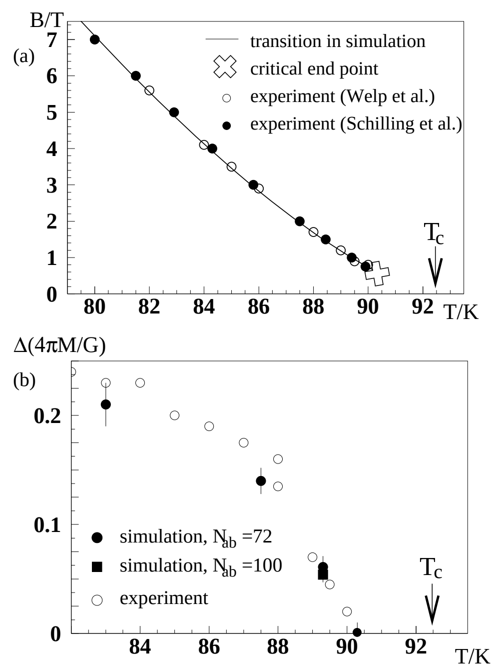

FIG. 1. Phase diagram (a) and magnetization discontinuity (b). Experimental data is taken from Ref. [2,4] (a) and [4] (b). $N_{ab} \equiv$ vortices per layer (for numbers of layers see text).

where $\mathbf{B}=\nabla\times\mathbf{A}$, which we shall take as constant and uniform. In first approximation $\alpha(T)=\alpha'(T-T_c)$ and $\beta_{2D}(T)$ is constant; $\alpha', \beta_{2D}, J>0$.

The model was simulated using Langevin (Model A) dynamics. The equation $\partial\psi/\partial t=-\Gamma\partial\mathcal{H}/\partial\psi^*+\eta$ was integrated numerically, using pseudo-random numbers to imitate the Gaussian white noise η, $\langle\eta^*\,\eta\rangle=2\Gamma\, k_BT\,\delta_r\delta_t$. We studied N_{ab} vortices per layer for N_c spherical layers (see Ref. [8] for details of spherical boundary conditions), each of thickness d_0 and spacing d and imposed periodic boundary conditions $\psi_1=\psi_{N_c+1}$. For each layer ψ is expanded in eigenstates of the squared momentum operator $(-i\hbar\nabla-2e\mathbf{A})^2$. We retain eigenstates belonging only to the lowest eigenvalue $2eB\hbar$, (the lowest Landau level (LLL) approximation) which is a useful procedure over a large portion of the vortex liquid regime [9]. The model then depends on only two dimensionless parameters [10]. The first one is the 2D effective temperature and field parameter for each layer, given by $\alpha_{2T}=(d_0h/2e\,\beta_{2D}B\,k_BT)^{1/2}\alpha_H$, with $\alpha_H=\alpha(T)+eB\hbar/m_{ab}$. The second, $\eta=J/|\alpha_H|$, controls the strength of the coupling between layers.

If the order parameter varies only slowly across the layers [5], the layered material behaves like a continuum with a mass anisotropy γ and $\beta=\beta_{2D}\times d/d_0$. The effective mass m_c in the c-direction can be expressed in terms of the layer coupling term: $\eta=\hbar^2\,/\,2m_cd^2|\alpha_H|$. In the continuum model of an anisotropic 3D type II superconductor, all thermodynamic properties of the sample depend on only one parameter $\alpha_T\propto\alpha_H$. With $\kappa=\sqrt{\beta/2\mu_0}\times m_{ab}/e\hbar$ we can express α_T in terms of measurable quantities as

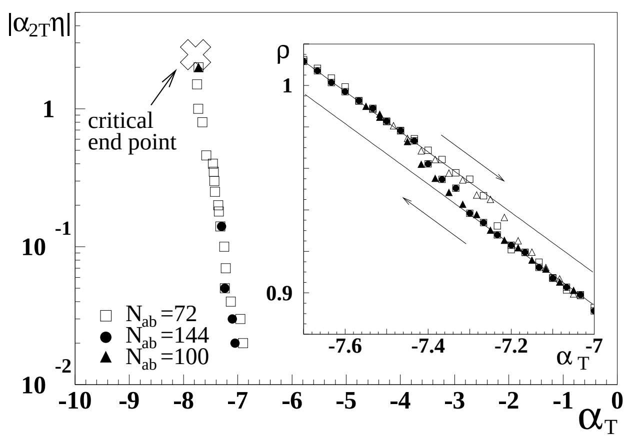

FIG. 2. First order transition points in the α_T–$|\alpha_{2T}\eta|$ plane. N_c varies between 8 and 80 for $|\alpha_{2T}\eta|$ between 0.02 and 2. The inset shows an example of the order parameter density ρ at constant $|\alpha_{2T}\eta|$, here $|\alpha_{2T}\eta|$=0.14, depending on increasing and decreasing α_T. Squares and triangles correspond to N_{ab}=72 and N_{ab}=144 respectively, filled symbols to cooling and open symbols to heating of the system. The transition is marked by a clear hysteresis loop. Solid lines mark the discontinuity in ρ.

$$\alpha_T=\left(\frac{\sqrt{2}\hbar^{3/2}\pi}{k_Be^{3/2}\mu_0}\right)^{2/3}\left(\frac{1}{\kappa^2\gamma}\right)^{2/3}\frac{\partial B_c/\partial T|_{T_c}(T-T_c)+B}{(BT)^{2/3}}.$$

Note that α_T=0 corresponds to the mean-field $H_{c2}(T)$ line and $\alpha_T=-\infty$ to T=0. The LD Hamiltonian reduces to the continuum Landau-Ginzburg model in the limit $\eta\to\infty$, $\alpha_{2T}\to0$, with $\alpha_T^3=\eta(2\alpha_{2T})^4$ fixed. Because YBCO is closer to being 3D rather than 2D in character, we shall quote results in terms of α_T rather than α_{2T}. The natural length scales of the continuum model are the magnetic length scale $l_m=\sqrt{\hbar/2eB}$, which is proportional to the vortex separation distance in the layers, and the mean field coherence length $\xi_{||}=\hbar/(2m_c|\alpha_H|)^{1/2}$ parallel to the field.

Instead of η we chose for our second independent parameter the product $|\alpha_{2T}\eta|$. Other than a factor $1/\sqrt{BT}$, $|\alpha_{2T}\eta|$ contains only material constants and therefore varies slowly for rather a wide range of α_H and over considerable regions of the B-T plane. For comparison with experiment, we can express the coupling strength as

$$|\alpha_{2T}\eta|=\left(\frac{\hbar^3\pi}{8e^3k_B\mu_0}\right)^{1/2}\frac{1}{\kappa\gamma^2d^{3/2}}\frac{1}{(BT)^{1/2}}.$$

Note that the (unknown) 2D parameters of the layers in the model, κ_{2D} and d_0, cancel from the the definition of $|\alpha_{2T}\eta|$ if the relation $\kappa=\sqrt{d/d_0}\times\kappa_{2D}$ is used. Thus we only need to know the value κ of bulk YBCO.

Fig. 2 shows the phase diagram in terms of simulation parameters. As $|\alpha_{2T}\eta|$ increases and the system approaches the continuum limit, the transition disappears at a critical point. This means that a first order transition is not expected to occur in superconductors such as niobium for which the continuum approximation is appropriate. Our simulation results imply that the end point of the first order transition in YBCO is intrinsically not an effect of disorder. (Recent experiments [11] show that its location is significantly shifted to higher fields, (which corresponds to lower coupling $|\alpha_{2T}\eta|$) in twinned samples. This effect could be interpreted as an effective enhancement of the correlations along the field direction by correlated disorder. We expect point disorder to have only a slight effect on the location of the end point). Note that along the transition line α_T is approximately constant, which means that the field and temperature dependence of the transition line behave like in a continuum model where α_T is the only scaling parameter in the system.

The inset of Fig.2 shows an example of the kind of measurement used to locate the first order transition. The system displays hysteresis at it upon heating and cooling and the effects of this on the order parameter density are shown. The order parameter density is given by $\rho=\alpha_T\,\beta/2\pi\alpha_H\times\langle|\psi|^2\rangle$. The magnetization in the LLL model is $4\pi M=(\mu_0e\hbar/m_{ab})\langle|\psi|^2\rangle$ (angular brackets signify a thermal average), which is in terms of our

simulation parameters $4\pi M = \pi(B - B_{c2}(T))\rho/\alpha_T \kappa^2$, where B is the applied magnetic field. Thus we can work out the magnetization discontinuity from the discontinuity in ρ at the transition. The data points in Fig.1(b) represent $|\alpha_{2T}\eta|$ =1, 1.5, 2 and 2.5 at N_c =50, 60, 60/80, 80. For these 4 transition points we have an average value of $\alpha_T = -7.72$, which yields the transition line in Fig.1(a). For $|\alpha_{2T}\eta|$=2 and $N_c d/\xi_{||} = 65$ we see a clear transition, while for $|\alpha_{2T}\eta|$=2.5 and $N_c d/\xi_{||} = 80$ there is no sign of a transition in the range $-8.3 < \alpha_T < -7.3$.

Near a critical end point we do not only expect the jump in the magnetization (order parameter density) to disappear, but we also expect there to be a divergence of the length scale of fluctuations in the order parameter density of the system. We therefore looked at the density-density correlations of the order parameter near the critical point. A normalized density-density correlator is $C_d(\Delta\mathbf{r}) = \langle|\psi(\mathbf{r})|^2|\psi(\mathbf{r}+\Delta\mathbf{r})|^2\rangle/\langle|\psi|^2\rangle^2 - 1$. Let us consider the case where $\Delta\mathbf{r}$ is a vector parallel to the c-axis. Plots of these correlations can be seen in Fig. 3. There is evidence of two length scales in the vicinity of the end-point. The short distance decay of the correlation function is dominated by the positional correlations of the vortices in the different layers. This length scale is mostly determined by α_T and changes slowly in the vicinity of the critical point. However a second longer length scale becomes visible between $\alpha_T = -7.6$ and $\alpha_T = -7.8$ as $|\alpha_{2T}\eta|$ is increased to its critical end point value. One can see in Fig. 3 that when $|\alpha_{2T}\eta|$ =2.5 and $\alpha_T = -7.8$ there is evidence of this much longer second length scale governing the decay of the correlation function at large distances. This length scale is associated with the density fluctuations at the critical end point and only become visible once it is larger than that of the vortex correlations. Due to the small amplitude of these density fluctuations very long simulation times are needed to determine the correlations within the statistical noise.

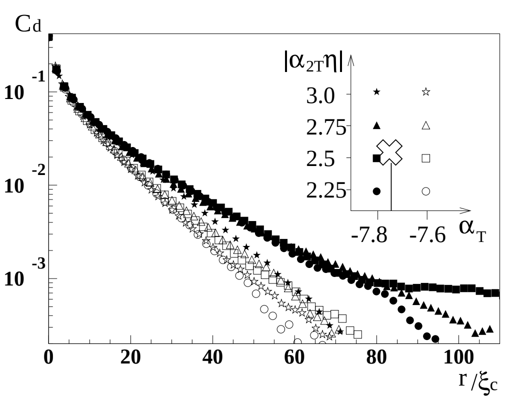

FIG. 3. Density-density correlations along the c-axis near the end the first order transition line and the critical point (see Inset). Note the decreasing difference in correlations between $\alpha_T = -7.6$ and $\alpha_T = -7.8$ as the transition disappears. For $|\alpha_{2T}\eta| = 2.5$ and $\alpha_T = -7.8$ we see evidence for a long length scale associated with fluctuations in the average order parameter density. System sizes are N_{ab}=72, $220 < N_c < 260$ for $\alpha_T = -7.6$ and $N_c = 270$ for $\alpha_T = -7.8$.

It is often supposed that the first order transition in YBCO changes to second order below the end point, where no latent heat is visible but a "step" in the heat capacity C remains [4,11]. We believe however that this "step" can be identified with the onset of a small peak in the superconducting specific heat $C_s = C - C_n$, (n for normal state), which is known to arise from thermal fluctuations. This peak has been observed for example in niobium by Farrant and Gough [12]. We find that the location and the height of the peak as well as the length of the rise (or width of the "step") in C from the low temperature value $C_{s,mf}$ (mf for mean field) to its maximum agree well for the niobium and YBCO measurements taken from Ref. [12] and [4]. The peak in C_s in niobium obeys LLL scaling [12] and is found at $\alpha_T/\beta_A = -6$, where $\beta_A = 1.16$, i.e. $\alpha_T \approx -7$. The data which shows the specific heat in YBCO is given as C minus $C(B = 0)$. The latter is near the "step" approximately equal to the low temperature value $C_{s,mf} + C_n$, so that the plotted quantity is approximately $C_s - C_{s,mf}$. The maximum occurs for example for $B = 0.25T$ at $T \approx 91.4$K which corresponds to $\alpha_T = -7.2$. The width of the "step" in niobium $\Delta\alpha_T \approx 2$. In YBCO for $B = 0.25T$ the specific heat rise associated with the step takes place in the temperature region $91 - 91.4K$, which corresponds to $\Delta\alpha_T = 2.8$. For niobium C_s is at its maximum 5% larger than $C_{s,mf}$. In YBCO we have to divide the plotted data by $C_{s,mf}$ to compare with this value. $C_{s,mf}$ is roughly given by the step in C at the zero field transition which we take from Ref. [4]. We find that $(C_s - C_{s,mf})/C_{s,mf} \approx 0.02$, which is of the same order as in niobium. The specific heat "step" in YBCO at different fields has approximately the same amplitude as well as width and position when expressed in terms of α_T, i.e. the "step" feature obeys LLL scaling. The quantitative agreement between YBCO and niobium strongly suggests that we are dealing with the same phenomenon and therefore that there really is no sharp specific heat step in YBCO.

The existence of the critical point implies that no symmetries are broken at the transition, which means it cannot be a liquid-crystal transition. We find indeed that the vortex matter is liquid on both sides of the transition. In Fig. 4 we show examples of density-density correlations above and below the transition for $|\alpha_{2T}\eta| = 1$ which corresponds to a transition temperature of 83 K in YBCO. Fig. 4(a) shows the correlations along the c-axis as previously seen in Fig. 3. We see an exponential decay of the correlation function with a finite length scale l_c for density correlations below as well as above the transition. Only for a liquid phase would this correlation function have an exponential decay. In Fig. 4(b) we show examples of measurements of the 2D Fourier transform of the density-density correlator C_d for $\Delta\mathbf{r}$ parallel to the lay-

ers, normalized by its high temperature limit, which is essentially the structure factor of the system (see Ref. [8] for details). It has its first and largest peak at the first reciprocal lattice vector of a triangular lattice, $k \approx 2.6$ in units of magnetic length. The inverse width at half maximum of the Lorentzian fits to this peak gives the length scale of crystalline order in the layers, l_{ab}. The length scales taken from fits in figure 4 are in order of decreasing α_T $l_c/\xi_{||}$ =13, 15, 20, 28, 46 and l_{ab}/l_m =1.33, 1.57, 1.94, 2.47, 2.73.

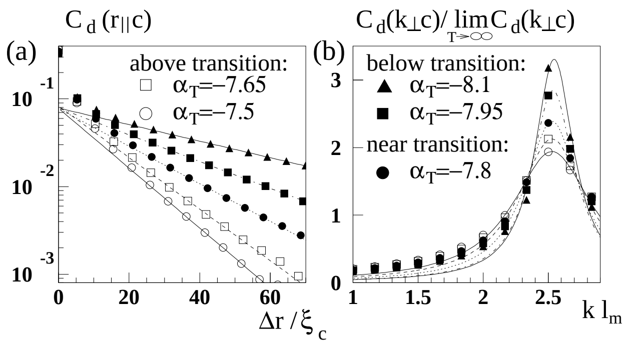

FIG. 4. (a) Density-density correlations along the c-axis (with linear fits), (b) structure factor (with Lorentzian fits) at $|\alpha_{2T}\eta|$=1. The system size is N_{ab}=72, N_c=270.

The length scales have a discontinuity at the transition. This jump is found to grow with distance from the end point, as one would naturally expect. We also see a rapid growth of the length scales below the transition. An exponential growth of length scales with $|\alpha_T|^{3/2} \sim (T_c - T)^{3/2}$, has been predicted for the low temperature regime from perturbative studies around zero temperature [6]. We can extrapolate the growth in the crystalline length scale obtained from Fig. 4 (b) just below the transition assuming exponential growth with $|\alpha_T|^{3/2}$. For a decrease of $\Delta\alpha_T \approx 1.2$, which corresponds in YBCO to cooling by only 1K below the transition at 83K, we obtain an increase in the range of crystalline order by a factor of 3. It is therefore likely that not far below the first order liquid-liquid transition length scales reach the system size in a pure system or in real crystals a "Larkin" like length scale (dependent on the amount of disorder present) so that the vortex liquid is correlated and effectively crystalline over large length scales. Although the structure factor in a liquid is rotationally symmetric, coupling with the underlying lattice may for long length scales lead to the appearance of Bragg–like peaks [13].

The longest time scales in the system, given by the decay of 3D Fourier component of C_d at the first reciprocal lattice vector in the *ab*-plane and k=0 along the *c*-axis (not shown), increase discontinuously across the transition. Such behavior may explain the sharp features of transport coefficients like resistivity. We also see extremely fast further growth of time scales below the transition in agreement with the fast decay of resistivity to zero as the temperature is lowered [10].

From previous simulations using the same model with periodic boundary conditions (PBC) in all directions instead of the geometry of spherical layers in a radial field, a vortex lattice melting transition is reported [14,15]. We find disagreement in the location of the transition due to the different choice of boundary conditions only for low $|\alpha_{2T}\eta|$. We believe that our choice of boundary conditions is more likely to reflect the real physics [16]. In the 3D-like regime appropriate to YBCO, the LLL-LD model may well show the same behavior for PBC as it does for spherical layers. For couplings high enough to see the critical point, the LLL-LD model has to our knowledge never been investigated using PBC. The largest system sizes used in the simulations with PBC are of the order of 40 vortices × 20 layers, smaller than the ranges of correlations we find below the transition. This would make the vortex liquid indistinguishable from a vortex lattice.

We have also attempted to compare our simulations with experimental data on $Bi_2Sr_2CaCu_2O_8$, for which the first order transition is in a region of the phase diagram where the LLL approximation is not good. As might be expected our results are not as quantitative as they are for YBCO but they are none the less still useful. Details will be given in [10].

In summary, we have found in a simulation the low field end point of the first order transition line in YBCO and obtained results in excellent agreement with experiment. The existence of a critical point implies that the vortex matter is liquid above and below the transition, and we were able to observe this directly in our simulation. Our results suggest that the transition in YBCO, which is commonly interpreted as vortex lattice melting, is of a liquid-liquid nature and that the vortex crystal state does not exist.

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